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## Investigation of Hydridosilsesquioxane-Based Silicon Oxide Deposition on Si(111)-7×7

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Beamline: U8B

**Introduction:** Knowledge of the structure and reactivity of the Si/SiO<sub>2</sub> interface is crucial to the continued scaling of microelectronic devices. As the gate oxide thickness decreases, the chemistry and physics occurring at the interface will begin to dominate the behavior of the devices. Assignment of the species present at the interface is complicated by its amorphous nature. The use of a well defined model system provides a framework for the assignment of structures present at the interface. One such model system, hydridosilsesquioxane clusters (HSiO<sub>3/2</sub>)<sub>n</sub>, has been studied in detail for Si(100)-2×1[1]. This work has now been extended to Si(111). Scanning tunneling microscopy (STM), X-ray photoemission spectroscopy (XPS), reflection absorption infrared spectroscopy (RAIRS), and low energy electron diffraction (LEED) have been used to characterize the reaction of octahydridosilsesquioxane (H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>) with the Si(111)-7×7 surface[2].

**Methods and Materials:** Octahydridosilsesquioxane (H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>) was synthesized by the method of Agaskar and sublimed twice[3]. XPS of the Si 2p core level and the valence band were obtained with an incident photon energy of 170 eV at beamline U8B at the NSLS. RAIRS, LEED, conventional XPS and STM were performed in a set of ultrahigh vacuum chambers at the University of Michigan. Clean Si(111)-7×7 surfaces were generated *in situ* by removal of the native oxide via resistive heating of the Si to ~1050 °C. Surfaces were checked for contamination by XPS or STM. The clean Si(111)-7×7 surfaces were then exposed to saturating doses of H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>.

**Results:** After exposure, the Si 2p core level is composed of features shifted 0 and -3.8 eV, relative to bulk Si. The feature at 0 eV is bulk Si, while the feature at -3.8 eV arises from the presence of HSiO<sub>3</sub> and SiO<sub>2</sub> moieties. In contrast to the reaction of H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub> with the Si(100)-2×1 surface, no features are observed at intermediate energies[1]. The valence band region for the reaction of H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub> with the Si(111)-7×7 surface more strongly resembles that of an amorphous siloxane than that of intact clusters. The RAIRS and LEED data also support the decomposition of the cluster on the surface. STM data reveals the formation of small islands on the Si(111) surface after exposure to H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>. In combination with the spectroscopic data, these islands are identified as silicon oxide. XPS and STM each indicate ~ 10% of the surface is covered by these islands. No intact clusters are observed on the surface. In contrast, STM images with internal resolution of intact clusters have been obtained for H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub> on Si(100)-2×1[4].

**Conclusions:** H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub> clusters decompose upon reaction with the Si(111)-7×7 surface to form silicon oxide islands. This decomposition is in stark contrast to the reaction of H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub> with the Si(100)-2×1 surface in which the clusters remain intact after chemisorption. The investigation of the reaction of H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub> with Si(111)-7×7 provides direct evidence of the spectroscopic signatures of decomposed H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub> clusters on Si surfaces.

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